A New Parameter and Evaluation Method for NIST-Modified UNIFAC

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The modified UNIFAC method is widely used for its convenience in process design and quick screening of alternatives in the early stage of process synthesis. A new method for evaluation of modified UNIFAC parameters is proposed, and evaluated group-group interaction parameters are presented. Newly evaluated parameter sets are called NIST-Modified UNIFAC parameters. The new method includes assessment of quality for VLE data which have been published previously, and uncertainty information of all mixture data sets (VLE, LLE, CPE, VE, SLE and HE) which have been implemented in TDE (Thermo DataEngine) developed by NIST. The concept of the parameter evaluation method and the current status of NIST-modified UNIFAC parameters are discussed.